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TITLE: Synthesis of tumor-inhibiting complex salts containing the anion trans-tetrachlorobis(indazole)ruthenate(III) and crystal structure of the tetraphenylphosphonium salt

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CORPORATE SOURCE: Institute General Inorganic Chemistry, Univ. Vienna, Vienna, A-1090, Austria

SOURCE: European Journal of Inorganic Chemistry (1999), (9), 1551-1555

CODEN: EJICFO; ISSN: 1434-1948

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Indazolium trans-tetrachlorobis(indazole)ruthenate(1-) exhibits excellent results against different tumor models in vitro and in vivo. To improve the water solubility necessary for the introduction of this tumor-inhibiting compound into clin. trials, the authors synthesized the corresponding Na salt in a 2-step ion exchange via the tetramethylammonium salt. The Na salt shows a 3,5-fold higher solubility in water relative to the indazolium salt. The authors also synthesized the n-butylammonium, n-octylammonium, and tetraphenylphosphonium salts, all of which showed improved solubility in organic solvents. The x-ray crystal structure of the latter could be solved, proving the trans configuration of the complex anion (triclinic, P.hivin.1, $a = 11.000(2)$, $b = 13.503(2)$, $c = 14.471(2)$ Å, $\alpha = 65.42(1)$, $\beta = 82.80(1)$, $\gamma = 67.93(1)^\circ$, $V = 1810.2$ Å³, $Z = 2$, $\rho_c = 1.50$ g/cm³, $\mu(\text{MoK}\alpha) = 8.1$, 5573 observed reflections with $F_o > 4\sigma(F_o)$, 562 refined parameters, $R1 = 0.033$, $wR2 = 0.088$). In spite of the paramagnetic Ru(III) center an assignment of the coordinated indazole protons could be made with the help of a COSY experiment

IT 124875-20-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant for preparation of tetraphenylphosphonium trans-tetrachlorobis(indazole)ruthenate(III))

RN 124875-20-3 CAPLUS

CN Ruthenate(1-), tetrachlorobis(1H-indazole- κ N2)-, (OC-6-11)-, hydrogen, compd. with 1H-indazole (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 124875-19-0

CMF C14 H12 Cl4 N4 Ru . H

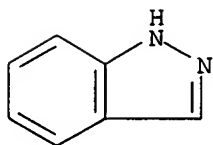
CCI CCS

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 271-44-3

CMF C7 H6 N2



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To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following: ME

Title of Invention: Compositions containing a ruthenium complex

Inventors (please provide full names): Keppeler et al

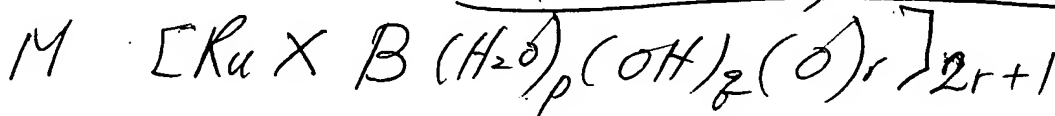
Earliest Priority Date: _____

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Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

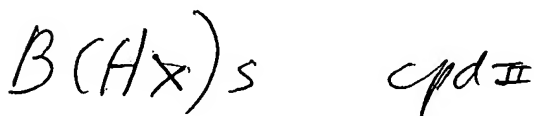
For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

I search compositions comprising cpd I, such as cpd I,
(see claim 33, & also see example I)



cpd I

* M is metal
X is halogen
HCO₃, R CO₂
(R is alkyl,
alkenyl)



* B is same as cpd I
X is same as cpd I
S is integer

* B is heterocycle,
ie. imidazole, pyrazole,
triazole, indazole

II process of making compositions and

* P, q, r = 0, 1, 2